EFD 03/08/200K

rior 1920 04/05/03.

10/551,998 Yong Chu 11-08-2007

\$%^STN;HighlightOn=;HighlightOff=;

Connecting via Winsock to STN

13/19 1026 - Cited

Smyther C.

Welcome to STN International! Enter x:x

LOGINID: ssptaylc1626

PASSWORD:

NEWS LOGIN

NEWS IPC8

TERMINAL (ENTER 1, 2, 3, OR ?):2

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Welcome to STN International
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NEWS
                 Web Page for STN Seminar Schedule - N. America
         JUL 02
NEWS
      2
                 LMEDLINE coverage updated
NEWS 3
         JUL 02
                 SCISEARCH enhanced with complete author names
NEWS 4 JUL 02
                 CHEMCATS accession numbers revised
NEWS 5 JUL 02 CA/CAplus enhanced with utility model patents from China
         JUL 16 CAplus enhanced with French and German abstracts
     6
NEWS
NEWS
      7
         JUL 18
                 CA/CAplus patent coverage enhanced
                 USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS
     8
         JUL 26
                 USGENE now available on STN
NEWS 9 JUL 30
         AUG 06 CAS REGISTRY enhanced with new experimental property tags
NEWS 10
         AUG 06
                 FSTA enhanced with new thesaurus edition
NEWS 11
        AUG 13 CA/CAplus enhanced with additional kind codes for granted
NEWS 12
                 patents
NEWS 13
         AUG 20
                 CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 14
         AUG 27
                 Full-text patent databases enhanced with predefined
                 patent family display formats from INPADOCDB
NEWS 15
         AUG 27
                 USPATOLD now available on STN
                 CAS REGISTRY enhanced with additional experimental
NEWS 16
         AUG 28
                 spectral property data
NEWS 17
         SEP 07
                 STN AnaVist, Version 2.0, now available with Derwent
                 World Patents Index
NEWS 18
         SEP 13
                 FORIS renamed to SOFIS
NEWS 19.
         SEP 13
                 INPADOCDB enhanced with monthly SDI frequency
NEWS 20
         SEP 17
                 CA/CAplus enhanced with printed CA page images from
                 1967-1998
         SEP 17
NEWS 21
                 CAplus coverage extended to include traditional medicine
                 patents
                 EMBASE, EMBAL, and LEMBASE reloaded with enhancements
         SEP 24
NEWS 22
NEWS 23
         OCT 02
                 CA/CAplus enhanced with pre-1907 records from Chemisches
                 Zentralblatt
NEWS 24
         OCT 19
                 BEILSTEIN updated with new compounds
              19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2,
NEWS EXPRESS
              CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.
              STN Operating Hours Plus Help Desk Availability
NEWS HOURS
```

Welcome Banner and News Items

For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 14:49:31 ON 08 NOV 2007

=> file reg

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 14:49:46 ON 08 NOV 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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STRUCTURE FILE UPDATES: 7 NOV 2007 HIGHEST RN 952647-77-7 DICTIONARY FILE UPDATES: 7 NOV 2007 HIGHEST RN 952647-77-7

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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http://www.cas.org/support/stngen/stndoc/properties.html

Uploading C:\Documents and Settings\ychu\Desktop\Case\10551998\10551998.str

chain nodes : 12 13 14

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

1-7 9-12 10-13 13-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11

exact/norm bonds :

1-7 7-8 7-11 8-9 9-10 10-11 13-14

exact bonds : 9-12 10-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

#### Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:CLASS 14:Atom

Generic attributes :

12:

Saturation

: Unsaturated

#### L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

Structure attributes must be viewed using STN Express query preparation.

0 ANSWERS

=> s l1

SAMPLE SEARCH INITIATED 14:50:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 6383 TO ITERATE

31.3% PROCESSED 2000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 122870 TO 132450

PROJECTED ANSWERS: 0 TO 0

=> s l1 full

FULL SEARCH INITIATED 14:50:11 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 128497 TO ITERATE

100.0% PROCESSED 128497 ITERATIONS

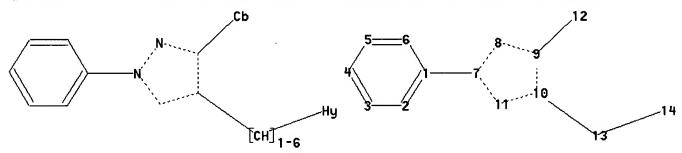
0 ANSWERS

SEARCH TIME: 00.00.02

L3 0 SEA SSS FUL L1

=>

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chain nodes : 12 13 14

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

1-7 9-12 10-13 13-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11

exact/norm bonds :

1-7 7-8 7-11 8-9 9-10 10-11 13-14

exact bonds :

9-12 10-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom

11:Atom 12:Atom 13:CLASS 14:Atom

Generic attributes :

12:

Saturation

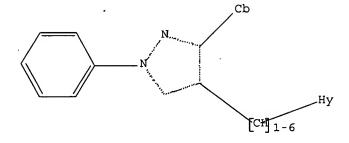
: Unsaturated

L4 STRUCTURE UPLOADED

=> d

L4 HAS NO ANSWERS

L4 STR



Structure attributes must be viewed using STN Express query preparation.

1 ANSWERS

=> s 14

SAMPLE SEARCH INITIATED 14:51:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 6383 TO ITERATE

31.3% PROCESSED 2000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 122870 TO 132450

PROJECTED ANSWERS: 1 TO 170

L5 1 SEA SSS SAM L4

=> s 14 full

FULL SEARCH INITIATED 14:51:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 128497 TO ITERATE

100.0% PROCESSED 128497 ITERATIONS 196 ANSWERS

SEARCH TIME: 00.00.02

L6 196 SEA SSS FUL L4

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 344.65 344.86

FILE 'CAPLUS' ENTERED AT 14:51:22 ON 08 NOV 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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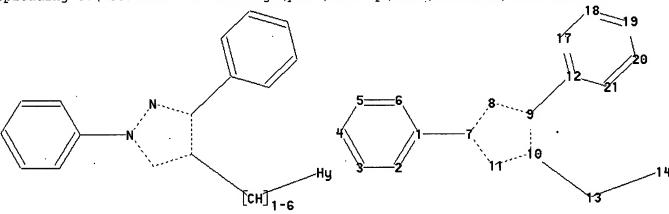
FILE COVERS 1907 - 8 Nov 2007 VQL 147 ISS 20. FILE LAST UPDATED: 7 Nov 2007 (20071107/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

### http://www.cas.org/infopolicy.html

=> s 16 L7 40 L6

=> Uploading C:\Documents and Settings\ychu\Desktop\Case\10551998\10551998B.str



chain nodes : 13 14 ring nodes : 7 8 9 10 11 12 17 18 19 20 21 1 2 3 4 5 6 chain bonds : 1-7 9-12 10-13 13-14 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11 12-17 12-21 17-18 18-19 19-20 20-21 exact/norm bonds : 1-7 7-8 7-11 8-9 9-10 10-11 13-14 exact bonds : 9-12 10-13 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 12-17 12-21 17-18 18-19 19-20 20-21

### Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom

## STRUCTURE UPLOADED

L8

Structure attributes must be viewed using STN Express query preparation.

=> s 18

· REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 14:54:51 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1722 TO ITERATE

100.0% PROCESSED 1722 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 31951 TO 36929 PROJECTED ANSWERS: 7 TO 298

L9 7 SEA SSS SAM L8

L10 6 L9

Uploading C:\Documents and Settings\ychu\Desktop\Case\10551998\10551998C.str

7 ANSWERS

chain nodes :

13

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 16 17 18 19 20 21 22 23 24 25 26

chain bonds :

1-7 9-12 10-13 13-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11 12-16 12-20 16-17 17-

18

18-19 19-20 21-22 21-26 22-23 23-24 24-25 25-26

exact/norm bonds :

 $1-7 \quad 7-8 \quad 7-11 \quad 8-9 \quad 9-10 \quad 10-11 \quad 13-21 \quad 21-22 \quad 21-26 \quad 22-23 \quad 23-24 \quad 24-25 \quad 25-26$ 

exact bonds :

9-12 10-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 12-16 12-20 16-17 17-18 18-19 19-20

### Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom

24:Atom 25:Atom 26:Atom

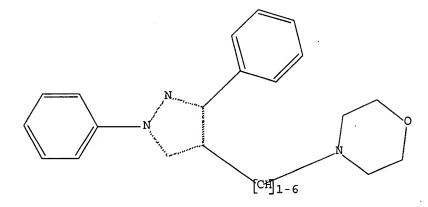
## L11 STRUCTURE UPLOADED

=> d

L11 HAS NO ANSWERS

L11

STR



Structure attributes must be viewed using STN Express query preparation.

=> s 111

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 14:56:38 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 47 TO ITERATE

47 ITERATIONS

100.0% PROCESSED SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\* 0 ANSWERS

PROJECTED ITERATIONS: 529 TO 1351

PROJECTED ANSWERS: OTO

0 SEA SSS SAM L11 L12

0 L12 L13

=> file reg

SINCE FILE COST IN U.S. DOLLARS TOTAL

SESSION ENTRY 0.47 350.46 FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 14:56:47 ON 08 NOV 2007 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2007 American Chemical Society (ACS)

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# http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Documents and Settings\ychu\Desktop\Case\10551998\10551998C.str

chain nodes :

13

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 16 17 18 19 20 21 22 23 24 25 26

chain bonds :

1-7 9-12 10-13 13-21

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11 12-16 12-20 16-17 17-

18-19 19-20 21-22 21-26 22-23 23-24 24-25 25-26

exact/norm bonds :

 $1-7 \quad 7-8 \quad 7-11 \quad 8-9 \quad 9-10 \quad 10-11 \quad 13-21 \quad 21-22 \quad 21-26 \quad 22-23 \quad 23-24 \quad 24-25 \quad 25-26$ 

exact bonds :

9-12 10-13

normalized bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 12-16 \quad 12-20 \quad 16-17 \quad 17-18 \quad 18-19 \quad 19-20$ 

Match level :

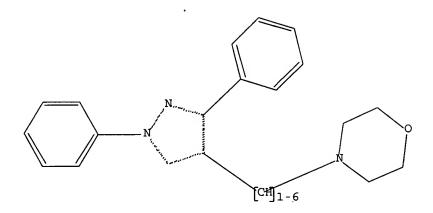
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom

22:Atom 23:Atom

24:Atom 25:Atom 26:Atom

#### L14 STRUCTURE UPLOADED

=> d L14 HAS NO ANSWERS L14 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 114

SAMPLE SEARCH INITIATED 14:57:11 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 47 TO ITERATE

100.0% PROCESSED 47 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 529 TO 1351
PROJECTED ANSWERS: 0 TO 0

L15 0 SEA SSS SAM L14

=> s 114 full

FULL SEARCH INITIATED 14:57:18 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 987 TO ITERATE

100.0% PROCESSED 987 ITERATIONS 9 ANSWERS

SEARCH TIME: 00.00.01

L16 9 SEA SSS FUL L14

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 172.10 522.56

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FILE COVERS 1907 - 8 Nov 2007 VOL 147 ISS 20 FILE LAST UPDATED: 7 Nov 2007 (20071107/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. No Gurat opp was found

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=> s 116

L17 3 L16

=> d ibib abs hitstr tot

L17 ANSWER 1 OF 3 CAPLUS COPTRIGHT 2007 ACS on STN 2007:642442 CAPLUS Full-text ACCESSION NUMBER:

DOCUMENT NUMBER:

147:72771

TITLE:

Preparation of morpholinecarboxamides as prokineticin

2 receptor antagonists

INVENTOR(S):

Thompson, Wayne J.; Melamed, Jeffrey Y.

PATENT ASSIGNED SOURCE:

Merck & Co., Inc., USA PCT Int. Appl., 100pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

. APPLICATION NO. KIND DATE PATENT NO. -------------------20070614 WO 2006-US46330 20061204 WO 2007067511 A2 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BY, CA, CH, CN, CO, CP, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, CB, CD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM US 2005-742770P P 20051206 PRIORITY APPLN. INFO.:

US 2006-830242P P 20060712

US 2006-856984P P 20061106

MARPAT 147:72771 OTHER SOURCE(S):

GI

AB Title compds. [I; A = Ph, naphthyl, heteroaryl; B = atoms to form (substituted) dioxanyl, pyranyl, cyclohexyl, Ph, pyridyl, etc.; X, Y = (substituted) alkylene; Rla, Rlb, Rlc = null, H, halo, OH, CO2H, cyano, NO2, (substituted) alkyl, alkoxy, alkoxycarbonyl, Ph, PhO, PhO2C, etc.; R2 = H, (substituted) alkyl, cycloalkyl, Ph], were prepd. Thus, title compd. (II) was prepd. in 3 steps from 1,3-dibromopropane, 3,5- dihydroxybenzaldehyde, isobutylamine, and 4-benzylmorpholine-2-carboxylic acid hydrochloride. I generally showed prokineticin 2 receptor antagonism with IC50 <10 .mu.M.

IT 941708-07-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compd.; prepn. of morpholinecarboxamides as prokineticin 2 receptor antagonists)

RN 941708-07-2 CAPLUS

CN 2-Morpholinecarboxamide, N-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]-4[(1,3-diphenyl-1H-pyrazol-4-yl)methyl]-N-(2-methylpropyl)- (CA INDEX NAME)

L17 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1997:757466 CAPLUS Full-text

DOCUMENT NUMBER: 128:88906

TITLE: A convenient one-pot synthesis of pyrazolo[3,4-

d]pyrimidines and s-triazolo[3,4-b][1,3,5]thiadiazines

AUTHOR(S): Hozden, Zeinab A.; Abd El-Wareth, A. O. Sarhan; El-Sherief, Hassan A. H.; Mahmoud, Abdalla M.

CORPORATE SOURCE: Chemistry Department, Faculty Science, Assiut

University, Assiut, 71516, Egypt

SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences

(1997), 52(11), 1401-1412

CODEN: ZNBSEN; ISSN: 0932-0776

PUBLISHER: Verlag der Zeitschrift fuer Naturforschung

DOCUMENT TYPE: LANGUAGE: Journal English

OTHER SOURCE(S):

CASREACT 128:88906

The reaction of 5-amino-3-aryl-1-phenylpyrazoles with H2CO and secondary amines in boiling EtOH gave the corresponding 4-alkylaminomethyl derivs. and bis(4-pyrazolyl)methanes as byproduct. Such reaction with primary aliph. and arom. amines at room temp. afforded 1,3,5-trisubstituted and 1,3,5,7-tetrasubstituted tetrahydropyrazolo[3,4-d]pyrimidines, resp., in good yield. Similarly, the Mannich reaction of 5-mercapto-3-phenyl-1,2,4-triazole with secondary amines in boiling EtOH or with primary arom. amines at room temp. gave 2-substituted aminomethyl derivs., while with primary aliph. amines, 4-toluidine, and 4-anisidine at room temp., and with other primary arom. amines in boiling EtOH 1,2,4-triazolo[3,4-b]thiadiazines were obtained.

IT 200939-36-2P 200939-38-4P 200939-39-5P

200939-40-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of pyrazolopyrimidines and triazolothiadiazines)

RN 200939-36-2 CAPLUS

CN 1H-Pyrazol-5-amine, 4-(4-morpholinylmethyl)-1,3-diphenyl- (CA INDEX NAME)

200939-38-4 CAPLUS

RN

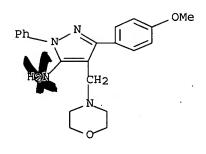
CN 1H-Pyrazol-5-amine, 3-(4-chlorophenyl)-4-(4-morpholinylmethyl)-1-phenyl-(CA INDEX NAME)

RN 200939-39-5 CAPLUS

CN 1H-Pyrazol-5-amine, 3-(4-methylphenyl)-4-(4-morpholinylmethyl)-1-phenyl-(CA INDEX NAME)

RN 200939-40-8 CAPLUS

CN 1H-Pyrazol-5-amine, 3-(4-methoxyphenyl)-4-(4-morpholinylmethyl)-1-phenyl-(CA INDEX NAME)



L17 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1974:108436 CAPLUS Full-text

DOCUMENT NUMBER: 80:108436

ORIGINAL REFERENCE NO.: 80817443a,17446a

TITLE: Reactions with 1,3-diphenyl-2-pyrazolin-5-one

AUTHOR(S): Sammour, A.; Abdel-Raouf, A.; Elkasaby, M.; Hassan, M.

Α.

CORPORATE SOURCE: Fac. Sci., Ain Shams Univ., Cairo, Egypt

SOURCE: E

Egyptian Journal of Chemistry (1972), 15(5), 429-44

CODEN: EGJCA3; ISSN: 0449-2285

DOCUMENT TYPE: Journal LANGUAGE: English

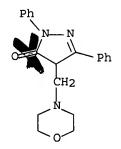
GI For diagram(s), see printed CA Issue.

AB 1,3-Diphenyl-2-pyrazolin-5-one I (R = H) (II) was condensed with aldehydes or ketones to give the pyrazolinones III (X = p-MeOC6H4CH, PhCH:CHCH, o-HOC6H4CH, Ph2C, etc.). II and p-RC6H4COCH:CHPh (R = H, MeO, Me) gave the pyrazolinones IV. II was treated with amines and HCHO to give I (R = piperidinomethyl, morpholinomethyl). III (X = p-MeOC6H4CH) with H2NCONH2 gave the oxazinopyrazole V and with H2NNH2 gave the pyrazolopyrazole VI.

IT 51813-63-9P 51813-69-5P

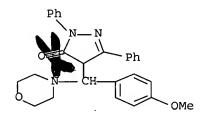
RN 51813-63-9 CAPLUS

CN 3H-Pyrazol-3-one, 2,4-dihydro-4-(4-morpholinylmethyl)-2,5-diphenyl- (9CI) (CA INDEX NAME)



RN 51813-69-5 CAPLUS

CN 3H-Pyrazol-3-one, 2,4-dihydro-4-[(4-methoxyphenyl)-4-morpholinylmethyl]-2,5-diphenyl- (9CI) (CA INDEX NAME)



=> file reg
COST IN U.S. DOLLARS

SINCE FILE ENTRY SI

TOTAL

FULL ESTIMATED COST

20.98

SESSION 543.54

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

CA SUBSCRIBER PRICE

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5=6 8. 9 12 21 20 14 13 14

chain nodes:

ring nodes :

 $1 \quad 2 \quad 3 \quad 4 \quad 5 \quad 6 \quad 7 \quad 8 \quad 9 \quad 10 \quad 11 \quad 12 \quad 17 \quad 18 \quad 19 \quad 20 \quad 21$ 

chain bonds :

1-7 9-12 10-13 11-23 13-14

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 7-8 \quad 7-11 \quad 8-9 \quad 9-10 \quad 10-11 \quad 12-17 \quad 12-21 \quad 17-18 \quad 18-18-19 \quad 18-19 \quad 18-$ 

19

19-20 20-21

exact/norm bonds :

1-7 7-8 7-11 8-9 9-10 10-11 11-23 13-14

exact bonds :

9-12 10-13

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 12-17 12-21 17-18 18-19 19-20 20-21

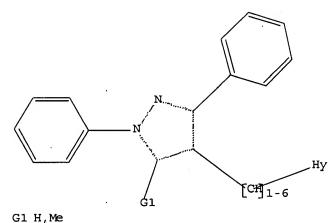
G1:H,CH3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 23:CLASS

L18 STRUCTURE UPLOADED

=> d L18 HAS NO ANSWERS L18 STR



01 11,12

Structure attributes must be viewed using STN Express query preparation.

6 ANSWERS

=> s 118

SAMPLE SEARCH INITIATED 15:04:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1722 TO ITERATE

100.0% PROCESSED 1722 ITERATIONS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 31951 TO 36929

PROJECTED ANSWERS: 6 TO 266

L19 6 SEA SSS SAM L18

=> s 118 full

FULL SEARCH INITIATED 15:04:32 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 34995 TO ITERATE

100.0% PROCESSED 34995 ITERATIONS 121 ANSWERS

SEARCH TIME: 00.00.02

L20 121 SEA SSS FUL L18

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 172.10 715.64

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE 0.00 -2.34

FILE 'CAPLUS' ENTERED AT 15:04:39 ON 08 NOV 2007
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=> s 120

L21 19 L20

=> d ibib abs hitstr tot

L21 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2007:652011 CAPLUS Full-text

DOCUMENT NUMBER: 147:27/504

TITLE: Genversion of some 2(3H)-furanones bearing a pyrazolyl

group into other heterocyclic systems with a study of

their antiviral activity

AUTHOR(S): Hashem, Ahmed I.; Youssef, Ahmed S. A.; Kandeel, Kamal

A.; Abou-Elmagd, Wael S. I.

CORPORATE SOURCE: Chemistry Department, Faculty of Science, Ain Shams

University, Cairo, Egypt

SOURCE: European Journal of Medicinal Chemistry (2007), 42(7),

934-939

CODEN: EJMCA5; ISSN: 0223-5234

PUBLISHER: Elsevier Masson SAS

DÖCUMENT TYPE: Journal LANGUAGE: English

GI

#### \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB 3-(1,3-Diphenylpyrazol-4-yl-methylene)-5-aryl-2(3H)-furanones I (R = H, Cl, OMe) were prepd. and converted into a variety of heterocyclic systems of synthetic and biol. importance. Benzylamine reacted with I; the product was found to depend on the reaction conditions. Thus, at room temp. the open-chain N-benzylamides were obtained, whereas under refluxing conditions the 2(3H)-pyrrolones II were obtained. Hydrazine hydrate affected ring opening of the furanones to give the corresponding acid hydrazides III. III were used as key starting materials for the synthesis of pyridazinones, 1,3,4-oxadiazoles, and 1,2,4-triazoles all bearing pyrazolyl moiety as a side-chain. Evaluation of antiviral activity of selected examples of the compds. obtained was performed using two viruses: HAV and HSV-1. Some of the tested compds. showed promising activities.

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (prepn. and antiviral activity of pyrazolylpyridazinones)

RN 946151-31-1 CAPLUS

CN 3(2H)-Pyridazinone, 4-[(1,3-diphenyl-1H-pyrazol-4-yl)methyl]-6-(4-methoxyphenyl)- (CA INDEX NAME)

IT 946151-25-3P 946151-28-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and antiviral activity of pyrazolylpyridazinones)

RN 946151-25-3 CAPLUS

CN 3(2H)-Pyridazinone, 4-[(1,3-diphenyl-1H-pyrazol-4-yl)methyl]-6-phenyl-(CA INDEX NAME)

RN 946151-28-6 CAPLUS

CN 3(2H)-Pyridazinone, 6-(4-chlorophenyl)-4-[(1,3-diphenyl-1H-pyrazol-4-yl)methyl]- (CA INDEX NAME)

L21 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2007 ACS ON STN

2007:642442 CAPLUS ACCESSION NUMBER:

NOT OPP, not in UI

DOCUMENT NUMBER:

147:72771

TITLE:

Preparation of morpholinecarboxamides as prokineticin

2 receptor antagonists

INVENTOR(S):

Thompson, Wayne J.; Melamed, Jeffrey Y.

PATENT ASSIGNEE(S):

Merck & Co., Inc., USA PCT Int. Appl., 100pp.

SOURCE:

CODENS PIXXD2

DOCUMENT TYPE: LANGUAGE:

Patent English

FAMILY ACC. NUM. COUNT

PATENT INFORMATION:

PATENT NO.				KIND		)	DATE		APPLICATION NO.						DATE		
					-												
WO 2007087511				A2		20070614		WO 2006-US46330						20061204			
	W : _	ÆΕ,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
	<b>3</b>	GE,	GH,	GM,	GT,	HN,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚĒ,	KG,	KM,	KN,
		KP,	KR,	KZ,	LA,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	LY,	MA,	MD,	MG,	MK,
		MN,	MW,	MX,	MY,	MZ,	NA,	NG,	NI,	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,
		RS,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SM,	SV,	SY,	TJ,	TM,	TN,	TR,	TT,
		TZ,	UA,	UG,	US,	UZ,	VC,	VN,	ZA,	ZM,	ZW						
	RW:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,
		IS,	IT,	LT,	LU,	LV,	MC,	NL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,
		CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG,	BW,	GH,
		GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	AM,	AZ,	BY,
		KG,	KZ,	MD,	RU,	TJ,	TM										
RITY APPLN. INFO.: US 2005-742770P													70P	P 20051206			

PRIORI

US 2006-830242P

US 2006-856984P

OTHER SOURCE(S):

MARPAT 147:72771

GI

Title compds. [I; A = Ph, naphthyl, heteroaryl; B = atoms to form AB (substituted) dioxanyl, pyranyl, cyclohexyl, Ph, pyridyl, etc.; X, Y = (substituted) alkylene; R1a, R1b, R1c = null, H, halo, OH, CO2H, cyano, NO2, (substituted) alkyl, alkoxy, alkoxycarbonyl, Ph, PhO, PhO2C, etc.; R2 = H, (substituted) alkyl, cycloalkyl, Ph], were prepd. Thus, title compd. (II) was prepd. in 3 steps from 1,3-dibromopropane, 3,5- dihydroxybenzaldehyde, isobutylamine, and 4-benzylmorpholine-2-carboxylic acid hydrochloride. I generally showed prokineticin 2 receptor antagonism with IC50 <10 .mu.M. 941708-07-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compd.; prepn. of morpholinecarboxamides as prokineticin 2 receptor antagonists)

RN 941708-07-2 CAPLUS

IT

CN 2-Morpholinecarboxamide, N-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]-4[(1,3-diphenyl-1H-pyrazol-4-yl)methyl]-N-(2-methylpropyl)- (CA INDEX NAME)

L21 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1190044 CAPLUS Full-text

DOCUMENT NUMBER: 146:142551

TITLE: Symphesis and anti-microbial activity of

AUTHOR(S): Sivaprasad, Ganesabaskaran; Perumal, Paramasivan T.; Prabavathy, Vaiyapuri R.; Mathivanan, Narayanasamy

CORPORATE SOURCE: Organic Chemistry Division, Central Leather Research

Institute, Chennai, 600 020, India

SOURCE: Bioorganic & Medicinal Chemistry Letters (2006),

16(24), 6302-6305

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:142551

GI

AB A series of pyrazolylbisindole derivs. have been synthesized by reacting substituted pyrazole aldehydes with substituted indoles using phosphotungstic acid, a Keggin type heteropoly acid as catalyst. The synthesized pyrazolylbisindoles were evaluated for their anti-microbial activities. The effect of pyrazolylbisindoles on the mycelial growth of plant pathogenic fungi was revealed. Compds. I (R = MeO or Br) emerged as the most interesting in this series exhibiting excellent anti-fungal activity.

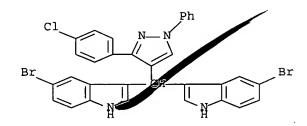
IT 918948-00-2P 918948-01-3P 918948-02-4P 918948-04-6P 918948-05-7P 918948-07-9P 918948-08-0P 918948-10-4P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. and antifungal activity of pyrazolylbisindoles via phosphotungstic acid-catalyzed coupling of substituted pyrazole aldehydes with substituted indoles)

RN 918948-00-2 CAPLUS

CN 1H-Indole, 3,3'-[[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis[5-bromo- (CA INDEX NAME)



RN 918948-01-3 CAPLUS

CN 1H-Indole, 3,3'-[[3-(4-methoxyphenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis[5-nitro- (CA INDEX NAME)

RN 918948-02-4 CAPLUS

CN 1H-Indole, 3,3'-[[3-(4-methoxyphenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis[5-bromo- (CA INDEX NAME)

RN 918948-04-6 CAPLUS

CN 1H-Indole, 3,3'-[[3-(4-bromophenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis[5-bromo- (CA INDEX NAME)

RN 918948-05-7 CAPLUS

CN 1H-Indole, 3,3'-[(1,3-diphenyl-1H-pyrazol-4-yl)methylene]bis[5-bromo- (CA INDEX NAME)

918948-07-9 CAPLUS

RN

CN 1H-Indole, 3,3'-[(1,3-diphenyl-1H-pyrazol-4-yl)methylene]bis[5-nitro- (CA INDEX NAME)

RN 918948-08-0 CAPLUS
CN 1H-Indole, 3,3'-[[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis[1-ethyl-2-phenyl- (CA INDEX NAME)

RN 918948-10-4 CAPLUS

CN 1H-Indole, 3,3'-[[3-(4-bromophenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis[1-ethyl-2-phenyl- (CA INDEX NAME)

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS
REFORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 4 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 2005:616664 CAPLUS Full-text

DOCUMENT NUMBER: 144:232969

TITLE: Synthesis of some 2-[2-(1,3-diphenyl-1H-pyrazol-4-

yl)vinylchromen-4-ones]

AUTHOR(S): Bachute, R. T.; Karale, B. K.; Gill, C. H.; Bachute,

M. T.

CORPORATE OURCE: P.G. Department of Chemistry, S.S.G.M. College,

Kopargaon, 423 601, India

SOURCE Indian Journal of Heterocyclic Chemistry (2005),

14(4), 375-376

CODEN: IJCHEI; ISSN: 0971-1627

PUBLISHER: Prof. R. S. Varma

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:232969

AB .beta.-Diketones are prepd. by B.V. transformation of the pyrazolylacrylic esters which in turn are obtained by esterification of the acrylic acids with 2-hydroxyacetophenones. The acid catalyzed cyclization of .beta.-diketones yielded 2-[2-(1,3-diphenyl-1H-pyrazol-4-yl)]vinylchromen- 4-ones and they showed moderate antibacterial activity.

IT 876749-73-4P 876749-74-5P 876749-75-6P

876749-76-7P 876749-77-8P 876749-78-9P

876749-79-0P 876749-80-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL

(Biological study); PREP (Preparation)

(prepn. and antimicrobial activity of 2-[2-(1,3-diphenyl-1H-pyrazol-4-yl)vinylchromen-4-ones] starting from pyrazolylacrylic acids and 2-hydroxyacetophenones)

RN 876749-73-4 CAPLUS

CN 4H-1-Benzopyran-4-one, 6-chloro-2-[2-[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl]ethenyl]- (CA INDEX NAME)

RN 876749-74-5 CAPLUS

CN 4H-1-Benzopyran-4-one, 6-chloro-2-[2-[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl]ethenyl]-7-methyl- (CA INDEX NAME)

RN 876749-75-6 CAPLUS

CN 4H-1-Benzopyran-4-one, 2-[2-[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl]ethenyl]-6-fluoro- (CA INDEX NAME)

RN 876749-76-7 CAPLUS

CN 4H-1-Benzopyran-4-one, 6-bromo-2-[2-[3-(4-chlorophenyl)-1-phenyl-1H-

pyrazol-4-yl]ethenyl]- (CA INDEX NAME)

RN 876749-77-8 CAPLUS

CN 4H-1-Benzopyran-4-one, 6-chloro-2-[2-[3-(4-methylphenyl)-1-phenyl-1H-pyrazol-4-yl]ethenyl]- (CA INDEX NAME)

RN 876749-78-9 CAPLUS

CN 4H-1-Benzopyran-4-one, 6-chloro-7-methyl-2-[2-[3-(4-methylphenyl)-1-phenyl-1H-pyrazol-4-yl]ethenyl]- (CA INDEX NAME)

RN 876749-79-0 CAPLUS

CN 4H-1-Benzopyran-4-one, 6,8-dimethyl-2-[2-[3-(4-methylphenyl)-1-phenyl-1H-pyrazol-4-yl]ethenyl]- (CA INDEX NAME)

RN 876749-80-3 CAPLUS

CN 4H-1-Benzopyran-4-one, 7-methyl-2-[2-[3-(4-methylphenyl)-1-phenyl-1H-pyrazol-4-yl]ethenyl]- (CA INDEX NAME)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 5 OF 19 CAPLUS COPYRIGHT 2007 ON STN
ACCESSION NUMBER: 2005:451965 CAPLUS Full-text

DOCUMENT NUMBER: 144:128892

TITLE: 4-Functionally-substituted 3-hetarylpyrazoles: Part

XV. 3-Acyl (hetaryl)-1-phenyl-4-pyrazolylmethylamines

and beterocumulenes obtained therefrom

AUTHOR(S): Bratenko, M. K.; Panimarchuk, O. I.; Mel'nichenko, N.

W.; Vovk, M. V.

CORPORATE SOURCE: Bukovinskaya State Medical Academy, Chernovtsy, 58000,

Ukraine

SOURCE: Russian Journal of Organic Chemistry (2005) 41(2),

238-242

CODEN: RJOCEQ; ISSN: 1070-4280

PUBLISHER: Pleiades Publishing, Inc.

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:128892

AB By redn. of 3-aryl(hetaryl)-1-phenyl-4-(azidomethyl)pyrazoles in the presence of Raney nickel or by hydrazinolysis of N-[3-aryl(hetaryl)-1- phenyl-4-pyrazolylmethyl]phthalimides, 4-pyrazolylmethylamines were obtained that in reaction with OC(OCCl3)2 afforded 3-aryl(hetaryl)-1- phenyl-4-pyrazolylmethyl isocyanates, and with CS2 furnished 3-aryl(hetaryl)-1-phenyl-4-pyrazolylmethyl isothiocyanates.

IT 873313-03-2P 873313-04-3P 873313-05-4P 873313-06-5P 873313-07-6P 873313-08-7P

873313-09-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of (arylpyrazolyl) methanamines)

RN 873313-03-2 CAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[(1,3-diphenyl-1H-pyrazol-4-yl)methyl]- (CA TNDEX NAME)

RN 873313-04-3 CAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[[3-(4-fluorophenyl)-1-phenyl-1H-pyrazol-4-yl]methyl]- (CA INDEX NAME)

RN 873313-05-4 CAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl]methyl]- (CA INDEX NAME)

RN 873313-06-5 CAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[[3-(3-bromophenyl)-1-phenyl-1H-pyrazol-4-yl]methyl]- (CA INDEX NAME)

RN 873313-07-6 CAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[[3-(4-bromophenyl)-1-phenyl-1H-pyrazol-4-yl]methyl]- (CA INDEX NAME)

RN 873313-08-7 CAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[[3-(4-methylphenyl)-1-phenyl-1H-pyrazol-4-yl]methyl]- (CA INDEX NAME)

RN 873313-09-8 CAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[[3-(4-methoxyphenyl)-1-phenyl-1H-pyrazol-4-yl]methyl]- (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 6 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

13

ACCESSION NUMBER:

CORPORATE SOURCE:

2004:755117 CAPLOS Full-text

DOCUMENT NUMBER:

142:178643

TITLE:

Synthesis and fastness properties of styryl and azo

disperse dies derived from 6-nitro substituted

3-aryl-20methyl-4(3H)-quinazolinone

AUTHOR(S):

Bhatti, Harjinder Singh; Seshadri, Sambamurthy
Dyes Research Laboratory, University Institute of

Chemical Technology, University of Mumbai, Mumbai,

400019, India

SOURCE:

Coloration Technology (2004), 120(4), 151-155

CODEN: CTOEAZ; ISSN: 1472-3581 Society of Dyers and Colourists

PUBLISHER:
DOCUMENT TYPE

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 142:178643

AB The synthesis of 6-nitro-substituted 3-aryl-2-methyl-4(3H)-quinazolinones from readily available starting materials, such as isatoic anhydride, is described. One of these, 3-phenyl-2-methyl-4(3H)-quinazolinone, has been utilized to prep. a range of styryl disperse dyes for polyester. Novel azo disperse dyes based on 6-nitro-3-[m-(diethylamino)phenyl]-2-methyl-4(3H)-quinazolinone as coupling component are reported. The application properties of the dyes on polyester and their fastness properties have been evaluated, with the latter being disappointing.

IT 834881-75-3P

RL: SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(dull yellow dye; prepn. and fastness properties of styryl and azo disperse dyes derived from quinazolinone)

RN 834881-75-3 CAPLUS

CN 4(3H)-Quinazolinone, 2-[2-(1,3-diphenyl-1H-pyrazol-4-yl)ethenyl]-6-nitro-3-phenyl- (CA INDEX NAME)

REFERENCE COUNT:

39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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2004:465425 CAPLUS Full-text ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE: Amberly 15 catalyzed synthesis of indole-pyrazole

based Fri (hetero) arylmethanes

Farhanullah; Sharon, Ashoke; Maulik, Prakas R.; Ram, AUTHOR (S):

ganu Ji

CORPORATE SOURCE: visions of Medicinal Chemistry, Central Drug

> esearch Institute, Lucknow, 226001, India Tetrahedron Letters (2004), 45(26), 5099-5102

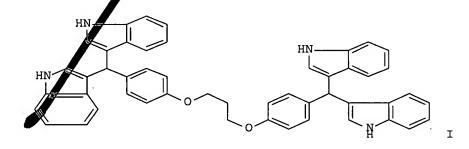
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier DOCUMENT TYPE: Journal English LANGUAGE:

OTHER SOURCE(S) CASREACT 141:207143

GI

SOURCE:



An expedient synthesis of 1,3-diaryl-4-(3,3'-diindolyl)methylpyrazoles has AB been developed using Amberlyst 15-catalyzed condensation of 1,3-diaryl-4formyl pyrazoles with indoles. This reaction was further extended to the synthesis of 4,4'-bis(3,3'-diindolyl)methylphenoxy-alkanes by coupling of 4,4'-di(formylphenoxy)alkane with indole. For example, the Amberlyst 15catalyzed condensation of 4,4'-[1,3- propanediylbis(oxy)]bis[benzaldehyde] with indole thus gave a (methylene)bis[1H-indole] deriv. (I) in 84% yield.

IT 741290-55-1P 741290-56-2P 741290-57-3P

741290-58-4P 741290-60-8P 741290-62-0P

741290-63-1P 741290-64-2P 741290-65-3P

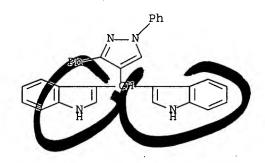
741290-66-4P 741290-67-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of [(pyrazolyl)methylene]bis[1H-indole] derivs. by Amberlyst 15-catalyzed condensation of indole with pyrazolecarboxaldehyde derivs.)

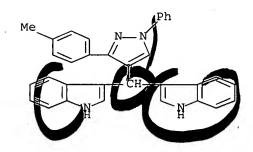
RN 741290-55-1 CAPLUS

CN 1H-Indole, 3,3'-[(1,3-diphenyl-1H-pyrazol-4-yl)methylene]bis- (CA INDEX NAME)



RN 741290-56-2 CAPLUS

CN 1H-Indole, 3,3'-[[3-(4-methylphenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis- (CA INDEX NAME)



RN 741290-57-3 CAPLUS

CN 1H-Indole, 3,3'-[[3-(4-methoxyphenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis- (CA INDEX NAME)

RN 741290-58-4 CAPLUS

CN 1H-Indole, 3,3'-[[3-(4-fluorophenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis- (CA INDEX NAME)

RN 741290-60-8 CAPLUS

CN 1H-Indole, 3,3'-[[3-(4-bromophenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis-(CA INDEX NAME)

RN 741290-62-0 CAPLUS

CN 1H-Indole, 3,3'-[(1,3-diphenyl-1H-pyrazol-4-yl)methylene]bis[2-phenyl-(CA INDEX NAME)

RN 741290-63-1 CAPLUS

CN 1H-Indole, 3,3'-[[3-(4-methylphenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis[2-phenyl- (CA INDEX NAME)

RN 741290-64-2 CAPLUS

CN 1H-Indole, 3,3'-[[3-(4-methoxyphenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis[2-phenyl- (CA INDEX NAME)

RN 741290-65-3 CAPLUS

CN 1H-Indole, 3,3'-[[3-(4-fluorophenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis[2-phenyl- (CA INDEX NAME)

RN 741290-66-4 CAPLUS

CN 1H-Indole, 3,3'-[[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis[2-phenyl- (CA INDEX NAME)

RN 741290-67-5 CAPLUS

CN 1H-Indole, 3,3'-[[3-(4-bromophenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis[2-phenyl- (CA INDEX NAME)

IT 741290-59-5P 741290-85-7P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. of [[(chlorophenyl)pyrazolyl]methylene]bis[1H-indole] and study of its crystal and mol. structures)

RN 741290-59-5 CAPLUS

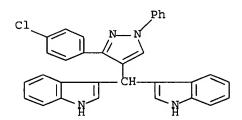
CN 1H-Indole, 3,3'-[[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis- (CA INDEX NAME)

RN 741290-85-7 CAPLUS

CN 1H-Indole, 3,3'-[[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl]methylene]bis-, compd. with trichloromethane (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 741290-59-5 CMF C32 H23 Cl N4



CM 2

CRN 67-66-3 CMF C H Cl3

C1 C1— CH— C1 L21 ANSWER 8 OF 19 CAPLUS COPYRIGHT 2001 ACS on STN

ACCESSION NUMBER: 2002:543324 CAPLUS Full-text

DOCUMENT NUMBER: 137:370022

TITLE: 4-Functionally Substituted 3-Heterylpyrazoles: VIII.

3-Aryl(heceryl)-4-hydroxyl(chloro)methylpyrazoles

AUTHOR(S): Bratenko, M. K.; Chornous, V. A.; Vovk, M. V.

CORPORATE SOURCE: Bukoyana State Medical Academy, Chernovtsy, 58000,

Ukraine

SOURCE: Rossian Journal of Organic Chemistry (Translation of

Zhurnal Organicheskoi Khimii) (2002), 38(3), 411-414

TT

CODEN: RJOCEQ; ISSN: 1070-4280

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S); CASREACT 137:370022

GI

AB 3-Aryl(heteryl)pyrazole-4-carbaldehydes were reduced with sodium borohydride under mild conditions to give 3-aryl(heteryl)-4- hydroxymethylpyrazoles, e.g., I, which were converted into the corresponding 4-chloromethyl derivs. by treatment with thionyl chloride. The subsequent reaction with triphenylphosphine led to formation of triphenyl(4-pyrazolylmethyl)phosphonium chlorides, and Wittig reaction of the latter with arom. or heteroarom. aldehydes yielded 4-[2-aryl(heteryl)ethenyl]pyrazoles, e.g., II.

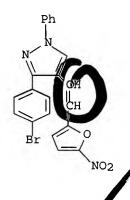
371773-67-0P 371773-80-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of arylethenyl(diaryl)pyrazoles via nucleophilic substitution of (diaryl)chloromethylpyrazoles with triphenylphosphine and subsequent Wittig reaction with arom. aldehydes)

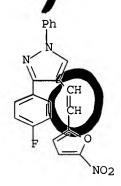
RN 371773-67-0 CAPLUS

CN 1H-Pyrazole, 3-(4-bromophenyl)-4-[2-(5-nitro-2-furanyl)ethenyl]-1-phenyl-(CA INDEX NAME)



RN 371773-80-7 CAPLUS

CN1H-Byrazole, 3-(4-fluorophenyl)-4-[2-(5-nitro-2-furanyl)ethenyl]-1-phenyl-CA INDEX NAME)



REFERENCE COUNT: THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS

RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

CAPLUS L21 ANSWER 9 OF 19 COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2000:10625 CAPLUS Full-text DOCUMENT NUMBER: 132:64186

Preparation of cyclic amidino agents useful as nitric TITLE:

oxide synthase inhibitors INVENTOR(S):

Hansen, Donald W., Jr.; Hallinan, E. Ann; Hagen, Timothy J.; Kramer, Steven W.; Metz, Suzanne;

Peterson, Karen B.; Spangler, Dale P.; Toth, Mihaly V.; Fok, Kam F.; Bergmanis, Arija A.; Webber, R.

Keith; Trivedi, Mahima; Tjoeng, Foe S.; Pitzele,

Barnett S.

PATEMP ASSIGNEE (S): G.D. Searle and Co., USA

SOURCE: U.S., 97 pp., Cont.-in-part of U.S. Ser. No. 425,831,

> abandoned. CODEN: USXXAM

DOCUMENT TYPE: Patent

English LANGUAGE: FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND .	DATE	APPLICATION NO.	DATE
US 6011028	A	20000104	US 1998-913838	19980327

WO 9633175

Al 19961024

WO 1996-US5315

19960419

W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI

RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN

PRIORITY APPLN. INFO.:

US 1995-425831 B2 19950420 WO 1996-US5315 W 19960419

OTHER SOURCE(S):

MARPAT 132:64186

GI

The current invention discloses useful amidino deriv. or general formula I [RI = (un) substituted cycloalkyl, heterocyclyl, aryl, etc; R2, R3, R4 = independently selected from H, alkyl, alkenyl, etc; R5, R6 = H, OH, or alkyloxy; A, B = alkyl, alkenyl, etc; L = alkylene, alkenylene, etc; a proviso is given; X = NH, O, S, alkyl, or alkenyl] useful as nitric oxide synthase inhibitors. Compd. II shows an IC50 value of 6.2.mu.M against human inducible nitric oxide synthase.

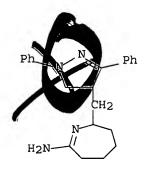
IT 184367-63-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of cyclic amidino agents useful as nitric oxide synthase

(prepn. of cyclic amidino agents useful as nitric oxide synthase inhibitors)

RN 184367-63-3 CAPLUS

CN 2H-Azepin-7-amine, 2-[(4,5-dihydro-1,3-diphenyl-1H-pyrazol-4-yl)methyl]-3,4,5,6-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)



HCl

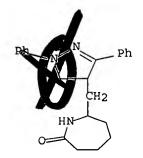
IT 253139-55-8P 253139-57-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of cyclic amidino agents useful as nitric oxide synthase inhibitors)

RN 253139-55-8 CAPLUS

CN 2H-Azepin-2-one, 7-[(4,5-dihydro-1,3-diphenyl-1H-pyrazol-4-yl)methyl]hexahydro- (CA INDEX NAME)



RN 253139-57-0 CAPLUS

CN 2H-Azepine, 2-[(4,5-dihydro-1,3-diphenyl-1H-pyrazol-4-yl)methyl]-3,4,5,6-tetrahydro-7-methoxy- (CA INDEX NAME)

REFERENCE COUNT:

1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 10 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1997:81434 CAPLUS Full-text

DOCUMENT NUMBER:

126:171499

TITLE:

1,3-Dipolar cycloadditions of electron-rich

benzotriazol-1-ylpropenes

AUTHOR(S): Katritzky, Alan R.; Musgrave, Richard P.; Breytenbach,

Jaco C.

CORPORATE SOURCE: Cent. Heterocyclic Compounds, Univ. Florida,

Gainesville, FL; 32611-7200, USA

SOURCE: Journal of Heterocyclic Chemistry (1996), 33(6),

1637-1646

CODEN: JHTCAD; ISSN: 0022-152X

PUBLISHER:

HeteroCorporation

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 126:171499

GI

The prepn. of trans-3-benzotriazol-1-yl-1-(N-morpholino)prop-1-ene, trans-3-benzotriazol-1-yl-1-ethoxyprop-1-ene, and trans-1,3-bis-(benzotriazol-1-yl)propene (I) and their reactions with benzonitrile oxide, N-(2,4-dibromophenyl)-1-phenylnitrilimine, and p-nitrophenyl azide are described. E.g., reaction of PhC.tplbond.N+O- with I, followed by refluxing in ethanolic HCl, gave isoxazole I (R = benzotriazol-1-yl).

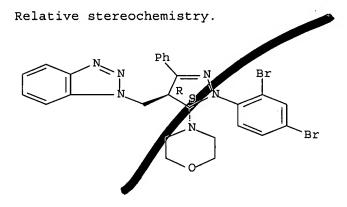
IT 187095-36-9P 187095-37-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(1,3-dipolar cycloaddns. of electron-rich benzotriazol-1-ylpropenes)

RN 187095-36-9 CAPLUS

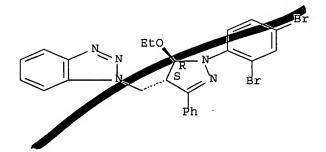
CN 1H-Benzotriazole, 1-[[1-(2,4-dibromophenyl)-4,5-dihydro-5-(4-morpholinyl)-3-phenyl-1H-pyrazol-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)



RN 187095-37-0 CAPLUS

CN 1H-Benzotriazole, 1-[[1-(2,4-dibromophenyl)-5-ethoxy-4,5-dihydro-3-phenyl-1H-pyrazol-4-yl]methyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



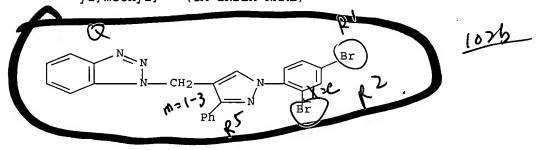
IT 187095-38-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(1,3-dipolar cycloaddns. of electron-rich benzotriazol-1-ylpropenes)

187095-38-1 CAPLUS RN

1H-Benzotriazole, 1-[[1-(2,4-dibromophenyl)-3-phenyl-1H-pyrazol-4-CN yl]methyl]-(CA INDEX NAME)



REFERENCE COUNT:

THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS 24 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 11 OF 19 APLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:55309 CAPLUS Full-text

DOCUMENT NUMBER: 126:199501

Design and synthesis of new triazole compounds TITLE:

containing 2H-pyrazole

AUTHOR (S): Shi, Yan-Nian; Yang, Yang; Fang, Jian-Xin; Lu,

Wen-Shuo

SOURCE: CORPORATE Inst. Elemento-Organic Chem., Nankai Univ., Tianjin,

300071, Peop. Rep. China

SOUR Gaodeng Xuexiao Huaxue Xuebao (1996), 17(10),

1578-1582

CODEN: KTHPDM; ISSN: 0251-0790.

PUBLISHER: Gaodeng Jiaoyu Chubanshe

DOCUMENT TYPE: Journal

LANGUAGE: Chinese GI

NPh I AB Title compds. I (R1 = Ph, 4-MeOC6H4, 4-ClC6H4, 3-O2NC6H4; R2 = Ph, 2-MeOC6H4, 4-MeOC6H4, 2-, 3-, 4-ClC6H4, 4-MeC6H4) were prepd. starting from reaction of R1COCH2CH2NMe2.HCl with triazole. I (R1 = Ph, R2 = 2-MeOC6H4) showed plant growth regulator activity.

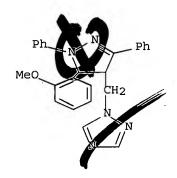
IT 186792-45-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis of pyrazolylmethyltriazoles as plant growth regulators)

RN 186792-45-0 CAPLUS

CN 1H-1,2,4-Triazole, 1-[[4,5-dihydro-5-(2-methoxyphenyl)-1,3-diphenyl-1H-pyrazol-4-yl]methyl]- (CA INDEX NAME)



IT 186792-44-9P 186792-46-1P 186792-47-2P

186792-48-3P 186792-49-4P 186792-50-7P

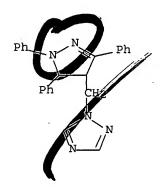
186792-51-8P 186792-52-9P 186792-53-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of pyrazolylmethyltriazoles as plant growth regulators)

RN 186792-44-9 CAPLUS

CN 1H-1,2,4-Triazole, 1-[(4,5-dihydro-1,3,5-triphenyl-1H-pyrazol-4-yl)methyl](CA INDEX NAME)



RN 186792-46-1 CAPLUS

CN 1H-1,2,4-Triazole, 1-[[4,5-dihydro-5-(4-methoxyphenyl)-1,3-diphenyl-1H-pyrazol-4-yl]methyl]- (CA INDEX NAME)

RN 186792-47-2 CAPLUS

CN 1H-1,2,4-Triazole, 1-[[5-(2-chlorophenyl)-4,5-dihydro-1,3-diphenyl-1H-pyrazol-4-yl]methyl]- (CA INDEX NAME)

RN 186792-48-3 CAPLUS

CN 1H-1,2,4-Triazole, 1-[[5-(3-chlorophenyl)-4,5-dihydro-1,3-diphenyl-1H-pyrazol-4-yl]methyl]- (CA INDEX NAME)

RN 186792-49-4 CAPLUS

CN 1H-1,2,4-Triazole, 1-[[5-(4-chlorophenyl)-4,5-dihydro-1,3-diphenyl-1H-pyrazol-4-yl]methyl]- (CA INDEX NAME)

RN 186792-50-7 CAPLUS

CN 1H-1,2,4-Triazole, 1-[[4,5-dihydro-5-(4-methylphenyl)-1,3-diphenyl-1H-pyrazol-4-yl]methyl]- (CA INDEX.NAME)

RN 186792-51-8 CAPLUS

CN 1H-1,2,4-Triazole, 1-[[4,5-dihydro-3-(4-methoxyphenyl)-1,5-diphenyl-1H-pyrazol-4-yl]methyl]- (CA INDEX NAME)

RN 186792-52-9 CAPLUS

CN 1H-1,2,4-Triazole, 1-[[3-(4-chlorophenyl)-4,5-dihydro-1,5-diphenyl-1H-pyrazol-4-yl]methyl]- (CA INDEX NAME)

RN 186792-53-0 CAPLUS

CN 1H-1,2,4-Triazole, 1-[[4,5-dihydro-3-(3-nitrophenyl)-1,5-diphenyl-1Hpyrazol-4-yl]methyl] - (CA INDEX NAME)

L21 ANSWER 12 OF 19

ACCESSION NUMBER:

DOCUMENT NUMBER:

TITLE:

INVENTOR(S):

SOURCE:

PATENT ASSIGNEE(S):

DOCUMENT TYPE:

LANGUAGE:

PATENT INFORMATION:

CAPLUS COPYRIGHT 2007 ACS on STN 1996:758969 CAPLUS Full-text 126:31278

PCT Int. Appl., 299 pp.

CODEN: PIXXD2

Preparation of iminoazepines and related cyclic amidines useful as nitric oxide synthase inhibitors. Hansen, Donald W., Jr.; Hallinan, E. Ann; Hagen, Timothy J.; Kramer, Steven W.; Metz, Suzanne; Peterson, Karen B.; Spangler, Dale P.; Toth, Mihaly V.; Fok, Kam F.; et al. G.D. Searle and Co., USA

Patent English FAMILY ACC. NUM. COUNT:

PATENT NO.				KIN	D	DATE		1	APPL	ICAT.	ION 1	. 00		D	ATE		
WO 9633175					Al 19961024			WO 1996-US5315						19960419			
7	W:	AL,	AM,	AT,	AU,	ΑZ,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CZ,	DE,	DK,	EE,
		ES,	FI,	GB,	GE,	HU,	IS,	JP,	KE,	KG,	KP,	KR,	KΖ,	LK,	LR,	LS,	LT,
	•	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,
		SG,	SI														
I	RW:	KE,	LS,	MW,	SD,	SZ,	ŪĠ,	AT,	BE,	CH,	DE,	DK,	ES,	FI,	FR,	GB,	GR,
		IE,	IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN.	
CA 22	216	882			A1		1996	1024		CA 1	996-	2216	882		1	9960	419

AU	9653916			Α	19961	107	AU	1996-53916	•	199604	119
UA	712315			B2	19991	104					
EP	821674			A1	19980	204	EP	1996-910833		199604	19
EP	821674			B1	20030	806					
	R: AT,	BE,	CH, I	DE,	DK, ES,	FR,	GB, GF	R, IT, LI, L	J, NL, S	SE, PT,	IE, FI
CN	1189823			Α	19980	805	CN	1996-194802		199604	19
CN	1105706			В	20030	416					
BR	9608012			A	19990	105	BR	1996-8012		199604	19
JP	11504319	)		T	19990	420	JP	1996-531885		199604	19
AT	246678			T	20030	815	AT	1996-910833		199604	19
ES	2206571			Т3	20040	516	ES	1996-910833		199604	119
TW	401401			В	20000	811	TW	1996-8510693	L5	199606	808
US	5883251			Α	19990	316	US	1997-977621		199711	125
US	6011028			A <sub>.</sub>	20000	104	US	1998-913838		199803	327
CN	1305993			A	20010	801	CN	2000-130981		200011	109
PRIORITY	APPLN.	INFO.	:				US	1995-425831	A2	199504	120
		•					WO	1996-US5315	W	199604	19

OTHER SOURCE(S):

MARPAT 126:31278

GI

AB Title compds. [I; R1 = (substituted) cycloalkyl, heterocyclyl, aryl; R2-R4 = H, (substituted) alkyl, alkenyl, alkynyl, OH, alkoxy, SH, alkylthio, amino, NO2, cyano, arylamino, alkylamino, acylamino, arylamino, haloalkyl, SO2NR7R9, etc.; R5, R6 = H, OH, alkoxy; R7 = H, alkyl, aryl; R8 = H, alkyl, COR9, CO2R9; R9 = alkyl, aryl; L = (substituted) alkylene, alkenylene, alkynylene, (CH2)mD(CH2)n; D = O, S, SO, SO2, SO2NR7, NR7SO2, NR8, POOR7, PON(R7)2, POOR7NR7, NR7POOR7, CO, CO2; B = (CH2)v, CH:CH; A = O, NR7, (CH2)q, CH:CH; X = CHNH, O, S, (CH2)p, CH:CH; m = 0-7; n = 0-5; p = 0-4; q = 1, 2], were prepd. Thus, 2-benzylcyclohexanone was converted to the oxime, which was heated in 80% aq. H2SO4 to give a mixt. of 3- and 7-benzylcaprolactam. The 7-benzyl isomer was treated with Me3OBF4 and mol. sieves to give the methoxyimine, which was refluxed with NH4Cl in MeOH to give title compd. (II). II inhibited human inducible nitric oxide synthase with IC50 = 6.2 .mu.M.

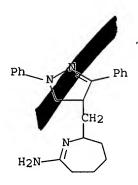
IT 184367-63-3P

> RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of iminoazepines and related cyclic amidines useful as nitric oxide synthase inhibitors)

184367-63-3 CAPLUS RN

CN 2H-Azepin-7-amine, 2-[(4,5-dihydro-1,3-diphenyl-1H-pyrazol-4-yl)methyl]-3,4,5,6-tetrahydro-, monohydrochloride (9CI) (CA INDEX NAME)



HC1

L21 ANSWER 13 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:502763 CAPLUS Full-text

DOCUMENT NUMBER: 123:143749

TITLE: A pericyclic cascade in the addition of diphenyl

nitrile imine to pyridine

AUTHOR(S): Caramella, Pierluigi; Gamba Invernizzi, Anna;

Pastormerlo, Eros; Quadrelli, Paolo; Corsaro, Antonino Dipartimento di Chimica Organica, Universita di Pavia,

CORPORATE SOURCE: Dipartimento di Chimica Organica, Pavia, I-27100, Italy

SOURCE: Heterocycles (1995), 40(2), 515-20

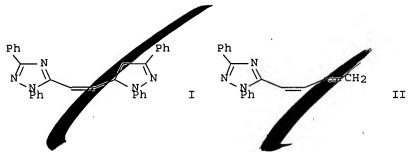
CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 123:143749

GI



On refluxing in benzene in the presence of excess pyridine the monocycloadduct of di-Ph nitrile imine to pyridine smoothly undergoes a [1,5] sigmatropic shift and a subsequent electrocyclic opening to afford 1,2,4-triazole derivs. I and II.

IT 165963-82-6P

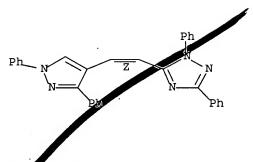
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(a pericyclic cascade in addn. of di-Ph nitrile imine to pyridine)

RN 165963-82-6 CAPLUS

CN 1H-1,2,4-Triazole, 5-[2-(1,3-diphenyl-1H-pyrazol-4-yl)ethenyl]-1,3-diphenyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



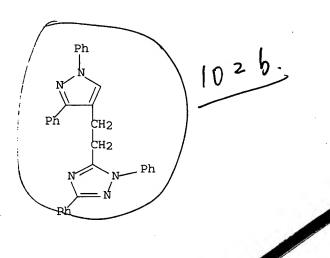
IT 165963-83-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(a pericyclic cascade in addn. of di-Ph nitrile imine to pyridine)

RN 165963-83-7 CAPLUS

CN 1H-1,2,4-Triazole, 5-[2-(1,3-diphenyl-1H-pyrazol-4-yl)ethyl]-1,3-diphenyl-(9CI) (CA INDEX NAME)



L21 ANSWER 14 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1993:256578 CAPLUS Full-text

DOCUMENT NUMBER: 118:256578

TITLE: Synthesis of arylpyrazolinylvinyloxazolidinodihydroind

oles and their chromophoric properties

AUTHOR(S): Ma, Yinmin; Li, Zhongjie

CORPORATE SOURCE: Dep. Chem., Northwest Univ., Xian, 710069, Peop. Rep.

China

SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1992), 13(10), 1262-4

CODEN: KTHPDM; ISSN: 0251-0790

DOCUMENT TYPE:

LANGUAGE:

Journal Chinese

OTHER SOURCE(S):

CASREACT 118:256578

AB The title dyes were synthesized by formylation of 1,5-diphenylpyrazoline, 1,3,5-triphenylpyrazoline, and 1,5-diphenyl-3-styrylpyrazoline with POCl3 in DMF, followed by condensation with 1-hydroxyethyl-2,3,3-trimethyl-3H- indolium iodide, and treatment with EtNa. The dyes were halochromic and piezochromic and thus suitable for manufg. acid-sensitive film and use as pressuresensitive pigments.

IT 148047-44-3P 148047-45-4P 148061-75-0P

148061-76-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. and chromophoric properties and applications of)

RN 148047-44-3 CAPLUS

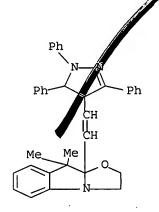
CN 3H-Indolium, 2-[2-(4,5-dihydro-1,3,5-triphenyl-1H-pyrazol-4-yl)ethenyl]-1-(2-hydroxyethyl)-3,3-dimethyl-, iodide (9CI) (CA INDEX NAME)

RN 148047-45-4 CAPLUS

CN 3H-Indolium, 2-[2-[4,5-dihydro-1,3-diphenyl-5-(2-phenylethenyl)-1H-pyrazol-4-yl]ethenyl]-1-(2-hydroxyethyl)-3,3-dimethyl-, iodide (9CI) (CA INDEX NAME)

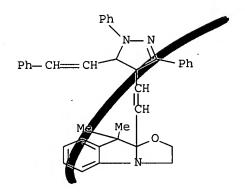
RN 148061-75-0 CAPLUS

CN Oxazolo[3,2-a]indole, 9a-[2-(4,5-dihydro-1,3,5-triphenyl-1H-pyrazol-4-yl)ethenyl]-2,3,9,9a-tetrahydro-9,9-dimethyl- (9CI) (CA INDEX NAME)



RN 148061-76-1 CAPLUS

CN Oxazolo[3,2-a]indole, 9a-[2-[4,5-dihydro-1,3-diphenyl-5-(2-phenylethenyl)-1H-pyrazol-4-yl]ethenyl]-2,3,9,9a-tetrahydro-9,9-dimethyl- (9CI) (CA INDEX NAME)



L21 ANSWER 15 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:122242 CAPLUS Full-text

DOCUMENT NUMBER: 114:122242

TITLE: Non-steroidal antiinflammatory agents. III: Synthesis

of pyrazole derivatives of 4(3H)-quinazolinones

AUTHOR(S): Farghaly, Ahmed M.; Chaaban, Ibrahim; Khalil, Mounir

A.; Bekhit, Adnan A.

CORPORATE SOURCE: Fac. Pharm., Univ. Alexandria, Alexandria, Egypt

SOURCE: Alexandria Journal of Pharmaceutical Sciences (1990),

4(1), 52-6

Journal

CODEN: AJPSES; ISSN: 1110-1792

DOCUMENT TYPE:

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:122242

GI

AB Several groups of compds. were synthesized having a pyrazole or pyrazoline moiety attached to 4(3H)-quinazolinone at the 2- or 3-position either directly or through different linkages. The linkages include methinamino, ethenyl, iminomethyl, aminomethyl or methinehydrazino grouping. Thus, acetanthranil (I) was treated with aminoantipyrine II to give 4(3H)-quinazolinone III. The antiinflammatory activity of representative examples of the products is reported.

IT 132088-52-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and antiinflammatory activity of)

RN 132088-52-9 CAPLUS

CN 4(3H)-Quinazolinone, 3-(4-chlorophenyl)-2-[2-[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl]ethenyl]- (9CI) (CA INDEX NAME)

RN 132088-46-1 CAPLUS
CN 4(3H)-Quinazolinome, 3-(4-methylphenyl)-2-[2-[3-(4-methylphenyl)-1-phenyl-1H-pyrazol-4-yl]ethenyl]- (9CI) (CA INDEX NAME)

RN 132088-47-2 CAPLUS
CN 4(3H)-Quinazolinone, 3-(4-bromophenyl)-2-[2-[3-(4-methylphenyl)-1-phenyl-1H-pyrazol-4-yl]ethenyl]- (9CI) (CA INDEX NAME)

RN 132088-48-3 CAPLUS

CN 4(3H)-Quinazolinone, 3-(4-chlorophenyl)-2-[2-[3-(4-methylphenyl)-1-phenyl-1H-pyrazol-4-yl]ethenyl] (9CI) (CA INDEX NAME)

RN 132088-49-4 CAPLUS

CN 4(3H)-Quinazolinore, 2-[2-[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl]ethenyl]-3-phenyl- (9CI) (CA INDEX NAME)

RN · 132088-50-7 CAPLOS

CN 4(3H)-Quinazolinone, 2-[2-[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl]ethenyl]-3-(4-methylphenyl)- (9CI) (CA INDEX NAME)

RN 132088-51-8 CAPLUS

'CN 4(3H)-Quinazolinone, 3-(4-bromophenyl)-2-[2-[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl]ethenyl]- (9CI) (CA INDEX NAME)

L21 ANSWER 16 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1989:431312 CAPLUS Full-text

DOCUMENT NUMBER:

111:31312

TITLE:

Electrophotographic photoreceptor containing azo

pigment carrier generator

INVENTOR(S):

Enomoto, Kazuhiro; Haino, Kozo

PATENT ASSIGNEE(S):

Mitsubishi Paper Mills, Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 20 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

LANGUAGE:

PE: Patent Japanese

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63309964	A	19881219	J# 1987-146510	19870611
JP 2506372	B2	19960612		
PRIORITY APPLN. INFO.:			JP 1987-146510	19870611
GI				
CpN = N $N - N$ $(CH = C)$	CH=(A)		≞NCp	

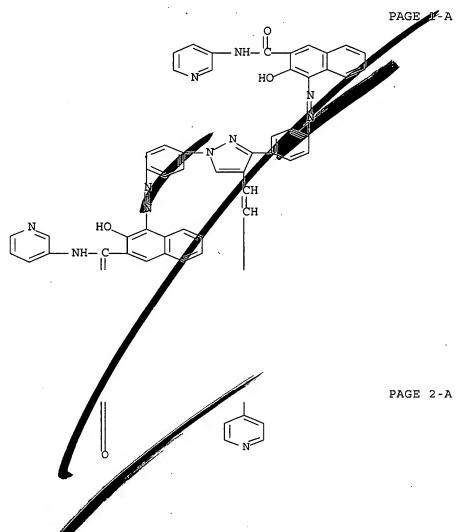
AB In the title photoreceptor, a photosensitive layer contains an azo pigment (I) [A = H, alkyl, aryl, hetero residue, carboxylic acid or its ester, cyano; X = H, cyano, halogen, lower alkyl, phenyl; m = 1, 2; n = 0, 1; Cp = coupler residue]. The photoreceptor shows improved heat and light resistances, and excellent carrier genation.

IT 121262-67-7

RL: USES (Uses)

(electrophotog. photoreceptor contg., as carrier generator)

CN 2-Naphthalenecarboxamide, 4,4'-[[4-[2-(4-pyridinyl)ethenyl]-1H-pyrazole-1,3-diyl]bis(4,1-phenyleneazo)]bis[3-hydroxy-N-3-pyridinyl- (9CI) (CA INDEX NAME)



L21 ANSWER 17 OF 29 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER 1984:220541 CAPLUS Full-text

DOCUMENT NUMBER: 100:220541

TITLE: Reactivity of Cu2(lonazolac)4, a lipophilic copper

acetate derivative

AUTHOR(S): Deuschle, Ulrich; Weser, Ulrich

CORPORATE SOURCE: Physiol.-Chem. Inst., Univ. Tuebingen, Tuebingen,

7400, Fed. Rep. Ger.

SOURCE: Inorganica Chimica Acta (1984), 91(4), 237-42

CODEN: ICHAA3; ISSN: 0020-1693

DOCUMENT TYPE: Journal LANGUAGE: English

AB Cu2L4 (HL = 3-(p-chlorophenyl)-1-phenylpyrazole-4-acetic acid) was prepd. and characterized. Cu in Cu2L4 was spin-coupled and remained EPR-silent. H2O and org. solvents did not affect this magnetic interaction. Superoxide dismutase activity of the Cu complex in micromolar concns. was detectable in the presence of <900 .mu.g per mL of serum albumin or whole serum protein. At 700 .mu.M albumin concn., a ternary complex between Cu2L4 and the protein was

formed. The original acetate-Cu coordination changed to a biuret-type Cu bonding as seen from EPR and electron absorption spectrometry. HL did not induce a detectable conformational change of the protein near or at the Cu binding site. Equil. dialysis and optical titrn. expts. revealed that essentially all Cu of Cu2L4 was bound in the specific binding site of serum albumin. The Cu complex proved to be an effective inhibitor of lipid peroxidn.

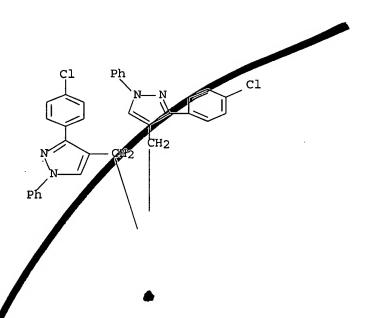
IT 90309-87-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn., superoxide dismutase activity and lipid peroxidn. inhibition by)

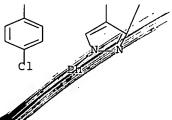
RN 90309-87-8 CAPLUS

CN Copper, tetrakis[.mu.-[3-(4-chlorophenyl)-1-phenyl-1H-pyrazole-4-acetato-0:0']]di-, (Cu-Cu) (9CI) (CA INDEX NAME)

PAGE 1-A



\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*



L21 ANSWER 18 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1974:552095 CAPLUS Full-text

PAGE 3-A

DOCUMENT NUMBER: 81:152095

ORIGINAL REFERENCE NO.: 81:23709a,23712a

Reactions of 4-[(1,3-diphenyl-4-pyrazolyl)methylene]-2-TITLE:

phenyl-2-oxazolin-5-one with Grignard reagents and

diazoalkanes

Elkaschef, Mohamed A. F.; Abdel-Megeid, Farouk M. E.; AUTHOR (S):

Yassin, Salah M. A.

Natl. Res. Cent., Cairo, Egypt CORPORATE SOURCE:

SOURCE: Journal fuer Praktische Chemie (Leipzig) (1974),

316(3), 363-8

CODEN: JPCEAO; ISSN: 0021-8383

DOCUMENT TYPE:

Journal English

LANGUAGE: GI For diagram(s), see printed CA Issue.

AB The title (pyrazolylmethylene) oxazolene I (Z = O) (II) reacted with excess RMqX (R = Ph, 4-MeOC6H4, Et, or PhCH2; X = Br or Cl) to give R1CH:C(NHBz)CR2OH and (or) I (Z = R2) or RR1CHCH(NHBz)COR. CH2N2 was added to II to give III (Z= O, R2 = H), whereas addn. of Ph2CN2 gave III (Z = CPh2, R2 = Ph).

IT 54294-60-9P 54294-61-0P

RL: SPN (Synthetic preparation) REPEP (Preparation)

(prepn. of)

RN 54294-60-9 CAPLUS

5(4H)-Oxazolone, 4-[1-(1,3-diphenyl-1H-pyrazol-4-yl)-2-hydroxyethyl]-4-hydroxy-2-phenyl- (9(1)) (CA INDEX NAME) CN

54294-61-0 CAPLUS

49[(1,3-diphenyl-1H-pyrazol-4-yl)hydroxymethyl]-4-CN 5(4H)-Oxazolone,

2 phenyl- (9CI) (CA INDEX NAME) (hydroxymethyl);

L21 ANSWER 19 OF 19 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1959:27685 CAPLUS

DOCUMENT NUMBER: 53:27685

ORIGINAL REFERENCE NO.: 53:4983i,4984a-i,4985a-c TITLE: Pyrazole cyanine dyes

INVENTOR(S): Kendall, John D.; Duffin, Geo. F.

PATENT ASSIGNEE(S): Ilford Ltd. DOCUMENT TYPE:

Patent

LANGUAGE:

AB

Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

GI For diagram(s), see printed CA Issue.

Pyrazole cyanine dyes are prepd. having the general formulas R1C:N.N(R).C(R2):CCH:CHC:N(R3)(X).D (I) or R1C:N.N(R).C(R2):CCH:C.C(:O).D1 (II), where R is an aryl group which may contain halogen, alkoxy, or acylamino substituents, and R1 and R2 are H, alkyl, or aryl groups, R3 is an alkyl group, X is an acid residue, D is the residue of a five- or six-membered heterocyclic N nucleus, and D1 is the residue of a five- or six-membered cyclic keto compd. I and II are prepd. by condensing a compd. of the general formula R1C:N.N(R).C(R2):CCHO (III) with a compd. of the general formula MeC:N(R3)(X).D (IV) or H2C.C(:O).D1 (V), preferably in the presence of a basic condensing agent, such as NaOAc or piperidine in EtOH or Ac2O. III are prepd. by treating a compd. of the general formula R1C:N.N(R).C(R2):CH (VI) with Nmethylformanilide and POCl3 and decompg. the mixt. with water. Thus, 1-(pchlorophenyl)-3,5-dimethylpyrazole (VII), a yellow oil, bl 119-26.degree., was prepd. from acetylacetone and p-chlorophenylhydrazine. p-Chlorophenylhydrazine 14.3 g., malonaldehyde tetramethyl acetal 16.4 g., and EtOH 50 ml. were refluxed; concd. HCl 12.5 ml. was added as rapidly as the exothermic reaction permitted. The mixt. was boiled for another 30 min. and dild. with water to ppt. an oil which rapidly solidified. The oil was dissolved in Et20 and the aq. liquors also extd. with ether. The combined Et2O solns. were washed with 2N HCl, dried with Na2SO4, and distd. to give 1-(p-chlorophenyl)pyrazole (VIII) a colorless solid, b0.5 108-10.degree., m. 52.degree.. Similarly were prepd.: 1-(2,5-dichlorophenyl)pyrazole (IX), paleyellow solid, m. 41.degree., b2 118-20; and 1-(p-methoxyphenyl)pyrazole (X), pale-yellow oil, b0.5 138-42.degree.. 3-Methyl-1-phenyl-2-pyrazoline 74 g., AcOH 465 ml., and Ac2O 280 ml: were heated to 55.degree. and red lead 325 g. added, with stirring, to the mixt. at such a rate as to keep the temp. at 75-80.degree.. The mixt. was then filtered, cooled, and dild. with EtOH, evapd. at 100.degree. and 25 mm. as far as possible, dild. with water, and extd. with Et2O. The Et2O soln. was washed with 2N HCl, water, and NaHCO3, dried over Na2SO4, and distd. to give 3-methyl-1-phenylpyrazole (XI) yellow oil, b15 135-40.degree.. 1,3-Diphenylpyrazole (XII), m. 83.degree. (from EtOH), was prepd. by a similar method. 1-Phenyl-3,5-dimethylpyrazole 17.2 g., Nmethylformanilide 18 g., and POCl3 12 cc. were refluxed on a water bath and after 20 min. dild. with a mixt. of cryst. NaOAc 110 g. and water 400 ml., and stirred for 1 hr. at room temp. The pptd. oil was extd. with Et2O (3 .times. 200 ml.) and the Et2O exts. washed with N HCl (3 .times. 100 ml.) and with dil. aq. NaHCO3. Evapn. of the ether left 1-phenyl-3,5-dimethylpyrazole-4carboxaldehyde (XIII), buff solid, m. 128.degree. (from MeOH). Analogously were prepd.: 1-phenylpyrazole-4-carboxaldehyde (XIV), colorless needles, m. 83.degree.; oxime m. 169.degree.; 1,3-diphenylpyrazole-4-carboxaldehyde (XV), m. 142.degree. (from EtOAc); 1-(p-chlorophenyl)pyrazole-4-carboxaldehyde (XVI), m. 118.degree. (from EtOH); 1-(2,5-dichlorophenyl)pyrazole-4carboxaldehyde (XVII), m. 114.degree. (from EtOH); 1-(pmethoxyphenyl)pyrazole-4-carboxaldehyde (XIX), m. 94.degree. (from C6H6); 3methyl-1-phenylpyrazole-4-carboxaldehyde (XX), m. 53.degree. (from cyclohexane); and 1-(p-chlorophenyl)-3,5-dimethylpyrazole-4-carboxaldehyde (XXI), m. 135.degree. (from EtOH). XV 1.11 g., 2,3,3-trimethylindolenine- MeI 1.32 g., anhyd. NaOAc 1.0 g., and EtOH 10 ml. were refluxed for 1 hr. The mixt. was then cooled, the pptd. solid filtered off, washed with water and EtOH, and recrystd. from MeOH to give 2-[2-(1,3 - diphenyl - 4 pyrazolyl)vinyl] - 1,3,3 - trimethylindoleninium iodide, orange-red leaflets,

decomp. 277.degree.. 2-Methylbenzothiazole (XIIIA) 0.61 g. and Et ptoluenesulfonate 0.81 g. were fused at 140-50.degree. for 3 hrs. XIV 0.7 g., EtOH 10 ml., and anhyd. NaOAc 1.0 g. were added and the mixt. refluxed for 1 hr. Diln. with water 80 ml. pptd. a solid, 3-ethyl-2-[2-(1-phenyl-4pyrazolyl)vinyl] benzothiazolium p-toluenesulfonate, yellow leaflets, m. 229-30.degree. (from water). Other pyrazole cyanines were prepd. similarly (components, color, and m.p. of product given): XIV, 2,3,3trimethylindolenine-MeI, orange, 245.degree. (from MeOH), XIV, quinaldine-EtI, orange, 247.degree. (from MeOH); XIII, 2-methylbenzothiazole-EtI, yellow, 217.degree. (decomp.) (from EtOH); 1,2,3,3-tetramethylindoleninium iodide, XVI, deep yellow, 250.degree.; XIV 1.72 g., 1-phenyl-3-methyl-5-pyrazolone 1.74 g., orange, 179.degree. (from C6H6); and quinaldine-MeI, XVI, orange, 249.degree.. Analogously, the following dyes were prepd. (product, color and m.p. given): 2-[2-(1-p-chlorophenyl - 4 - pyrazolyl)vinyl] - 3 ethylbenzothiazolium iodide, yellow, 260-1.degree.; chloride, yellow, 251.degree. (decomp.) (from MeOH); 2-[2-(1-p-chlorophenyl-4-pyrazolyl)vinyl]-3-ethylbenzoxazolium iodide, orange, 231.degree. (from MeOH). 2 - {2 - [1 -(2,5 - Dichlorophenyl) - 4 - pyrazolyl]vinyl} - 3 - ethylbenzothiazolium iodide orange, 230.degree. (decomp.) (from EtOH); chloride, yellow, 231.degree. (from EtOH);  $2-\{2-[1-(2,5-dichlorophenyl)-4-pyrazolyl]vinyl\}$ - 1,3,3-trimethylindoleninium iodide, orange, 173.degree. (from EtOH); 5 chloro - 2 - {2 - [1 - (2,5 - dichlorophenyl) - 4 - pyrazolyl]vinyl}-3ethylbenzothiazolium iodide, yellow-green, 205.degree. (from EtOH); 5-chloro-2-[2-(1-p-chlorophenyl-4-pyrazolyl)vinyl]-3- ethylbenzothiazolium iodide, orange, 238.degree. (decomp.) (from EtOH); 6,7-benzo-2-[2-(1-p-chlorophenyl-4pyrazolyl)vinyl]-3- methylbenzothiazolium p-toluenesulfonate, orange, 181.degree. (from EtOH); 2-[2-(1-p-chilorophenyl-3,5-dimethyl - 4 pyrazolyl)vinyl] - 3 - ethylbenzotbiazolium p-toluenesulfonate, yellow, 186.degree. (from water); 5-chloro-2-[2 - (1 - p - chlorophenyl - 3,5 dimethyl - 4 - pyrazolyl)vinyl 3-ethylbenzothiazolium p-toluenesulfonate, yellow, 228.degree. (from wager); 3-ethyl-2-[2-(3-methyl-1-phenyl-4pyrazolyl)vinyl]benzothiazofium iodide, orange, 255.degree. (from MeOH); 3ethyl-2-{2-[1-(p-methoxyphenyl)-4-pyrazolyl]vinyl}benzothiazolium iodide, orange, 260.degree. (decemp.); and 3-ethyl-5-[(1-phenyl-4pyrazolyl)methylene]-2-thiothiazolid-4-one, yellow, 236.degree. (from C6H6). 123885-63-2P, 2-[2-(1,3-Diphenylpyrazol-4-yl)vinyl]-1,3,3trimethyl-3H-indolium iodide RL: PREP (Preparation) (prepn. of)

RN 123885-63-2 CAPLUS

2-[2-(1,3-Diphen: Tpyrazol-4-yl)vinyl]-1,3,3-trimethyl-3H-indolium iodide CN (CA INDEX NAME)

IT

Executing the logoff script...

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	ENTRY	SESSION
CA SUBSCRIBER PRICE	-14.82	-17.16

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